



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:04 pm GMT

PDB ID : 4KSZ  
Title : Crystal structure of bovine lactoperoxidase complexed with cystiene at 1.98Å resolution  
Authors : Singh, R.P.; Singh, N.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2013-05-19  
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

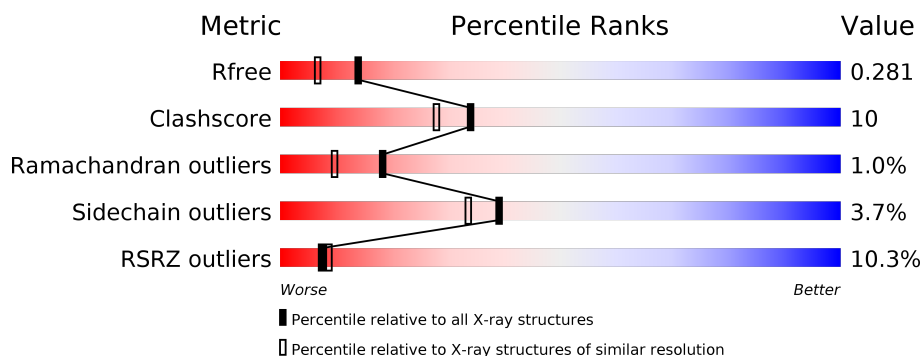
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	<div> <div>10%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	618	-	-	-	X
8	CYS	A	620	-	-	X	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5209 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

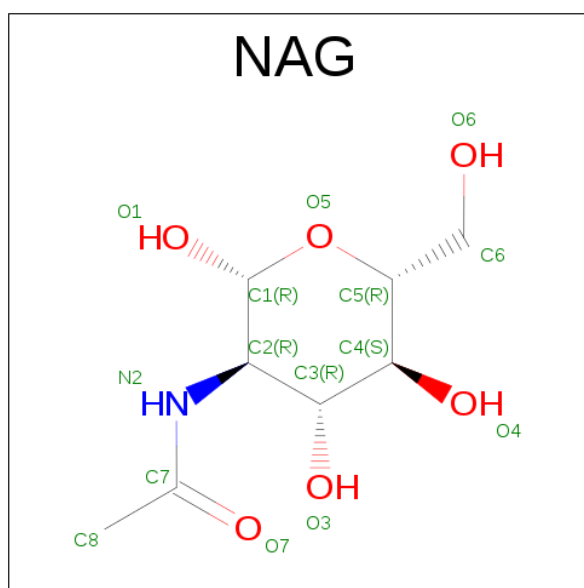
- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total I 11 11	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

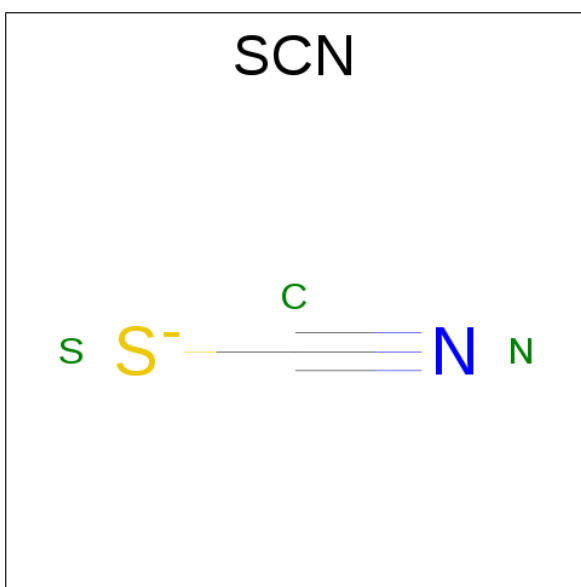
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



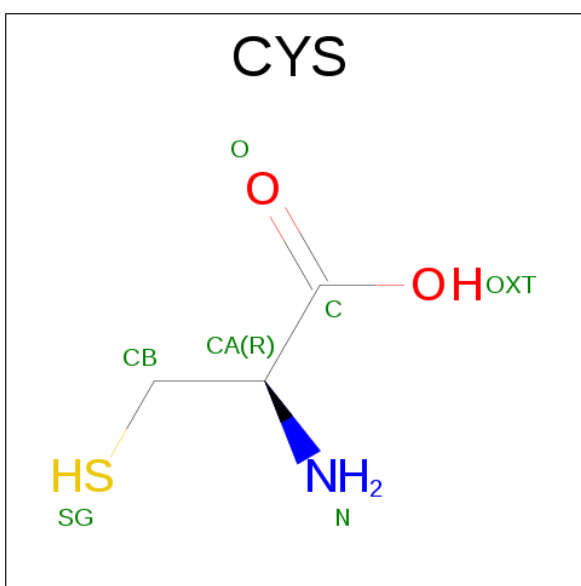
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 8 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

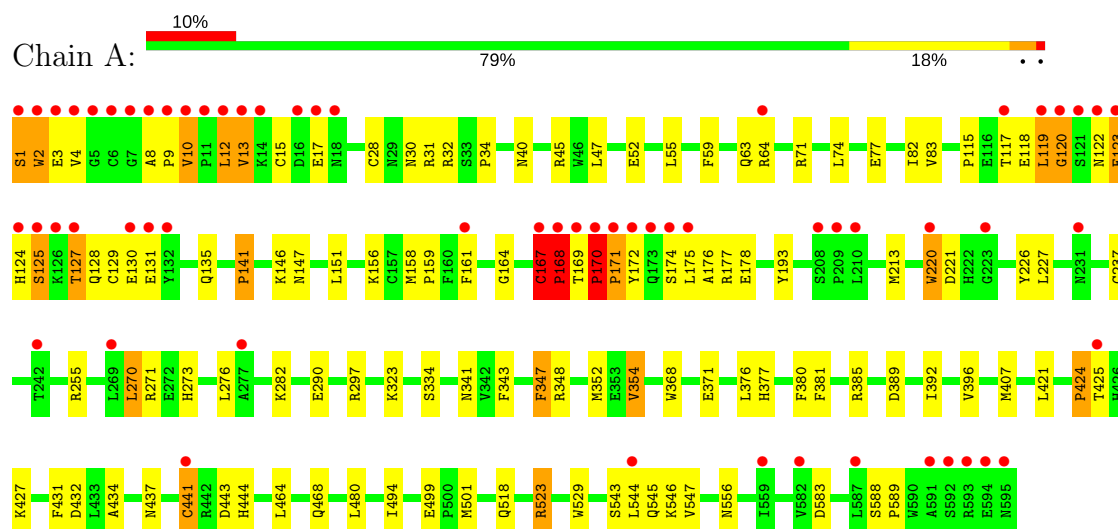
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	297	Total 297	O 297	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.01Å 80.30Å 76.51Å 90.00° 102.02° 90.00°	Depositor
Resolution (Å)	74.83 – 1.98 74.83 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (74.83-1.98) 96.7 (74.83-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.217 , 0.252 0.234 , 0.281	Depositor DCC
$R_{free}$ test set	2181 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, HEM, IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.08	10/4891 (0.2%)	1.03	19/6634 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	ALA	CA-CB	6.75	1.66	1.52
1	A	499	GLU	CD-OE2	-6.40	1.18	1.25
1	A	178	GLU	CB-CG	6.10	1.63	1.52
1	A	59	PHE	CD2-CE2	5.85	1.50	1.39
1	A	167	CYS	N-CA	5.84	1.58	1.46
1	A	220	TRP	CB-CG	-5.69	1.40	1.50
1	A	441	CYS	CB-SG	-5.45	1.73	1.81
1	A	354	VAL	CB-CG1	5.41	1.64	1.52
1	A	499	GLU	CD-OE1	-5.17	1.20	1.25
1	A	28	CYS	CB-SG	-5.08	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	C-N-CD	-12.26	93.64	120.60
1	A	168	PRO	N-CA-C	10.66	139.81	112.10
1	A	125	SER	CA-C-N	-9.03	97.33	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	PRO	CA-C-N	-7.66	100.36	117.20
1	A	169	THR	N-CA-C	6.73	129.16	111.00
1	A	125	SER	O-C-N	6.28	132.74	122.70
1	A	167	CYS	N-CA-C	-6.14	94.41	111.00
1	A	119	LEU	C-N-CA	5.97	134.83	122.30
1	A	10	VAL	C-N-CD	5.67	140.30	128.40
1	A	494	ILE	CG1-CB-CG2	-5.61	99.06	111.40
1	A	13	VAL	CB-CA-C	-5.56	100.84	111.40
1	A	443	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	125	SER	C-N-CA	5.52	135.51	121.70
1	A	523	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	177	ARG	CB-CG-CD	-5.50	97.29	111.60
1	A	45	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	47	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	523	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	13	VAL	CA-C-N	5.04	128.29	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	SER	Peptide
1	A	167	CYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4685	90	0
2	A	43	0	30	4	0
3	A	1	0	0	0	0
4	A	11	0	0	1	0
5	A	28	0	25	0	0
6	A	42	0	39	0	0
7	A	6	0	0	0	0
8	A	7	0	4	4	0
9	A	297	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5209	0	4783	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:HB2	1:A:171:PRO:CD	1.73	1.18
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.39	1.00
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.41	0.99
1:A:115:PRO:HG3	1:A:119:LEU:HD13	1.45	0.98
1:A:130:GLU:HA	1:A:159:PRO:HG3	1.58	0.85
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.58	0.83
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.05	0.82
1:A:407:MET:HB3	1:A:501:MET:CE	2.09	0.81
1:A:407:MET:HB3	1:A:501:MET:HE2	1.63	0.81
1:A:129:CYS:CB	1:A:161:PHE:HE1	1.97	0.77
1:A:127:THR:HG23	1:A:129:CYS:H	1.48	0.76
1:A:170:PRO:CB	1:A:171:PRO:CD	2.46	0.75
1:A:55:LEU:HD22	1:A:174:SER:H	1.52	0.73
1:A:115:PRO:CG	1:A:119:LEU:HD13	2.20	0.70
1:A:271:ARG:HG2	4:A:612:IOD:I	2.63	0.69
1:A:167:CYS:N	1:A:168:PRO:HD3	2.08	0.69
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.15	0.69
1:A:271:ARG:HB3	1:A:556:ASN:OD1	1.95	0.67
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.78	0.66
1:A:127:THR:HG23	1:A:129:CYS:N	2.10	0.66
1:A:129:CYS:HB3	1:A:161:PHE:HE1	1.60	0.65
1:A:255:ARG:HG2	8:A:620:CYS:HB3	1.77	0.64
1:A:543:SER:OG	1:A:589:PRO:HG2	1.99	0.63
1:A:464:LEU:O	1:A:468:GLN:HG3	1.99	0.62
1:A:352:MET:SD	1:A:407:MET:SD	2.97	0.62
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.35	0.62
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.30	0.61
1:A:129:CYS:HB3	1:A:161:PHE:CE1	2.35	0.60
1:A:129:CYS:SG	1:A:161:PHE:CE1	2.97	0.57
2:A:601:HEM:HBC2	2:A:601:HEM:HMC1	1.86	0.57
1:A:10:VAL:HG12	1:A:12:LEU:N	2.19	0.57
1:A:3:GLU:HG3	1:A:4:VAL:N	2.20	0.56
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.41	0.55
1:A:129:CYS:CB	1:A:161:PHE:CE1	2.86	0.55
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.42	0.55
1:A:10:VAL:CG1	1:A:12:LEU:HB2	2.37	0.55
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.42	0.54
1:A:13:VAL:HG12	1:A:13:VAL:O	2.07	0.53
1:A:146:LYS:O	1:A:147:ASN:CB	2.59	0.51
1:A:385:ARG:O	1:A:389:ASP:HB3	2.10	0.50
1:A:129:CYS:SG	1:A:161:PHE:HE1	2.35	0.50
1:A:175:LEU:HD23	1:A:176:ALA:O	2.12	0.49
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.59	0.49
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.49
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.49
1:A:82:ILE:CD1	1:A:480:LEU:HD23	2.42	0.49
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.93	0.49
1:A:341:ASN:OD1	1:A:444:HIS:ND1	2.33	0.49
1:A:17:GLU:HG2	1:A:31:ARG:HG2	1.95	0.49
1:A:158:MET:HE1	1:A:432:ASP:H	1.77	0.49
1:A:3:GLU:HG3	1:A:4:VAL:H	1.78	0.49
1:A:545:GLN:HG3	1:A:545:GLN:O	2.12	0.49
1:A:146:LYS:O	1:A:147:ASN:HB2	2.14	0.47
1:A:10:VAL:C	1:A:12:LEU:H	2.17	0.46
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.50	0.46
1:A:118:GLU:C	1:A:120:GLY:H	2.19	0.46
1:A:546:LYS:HB3	1:A:583:ASP:HB3	1.97	0.46
1:A:30:ASN:O	1:A:34:PRO:HA	2.16	0.45
1:A:128:GLN:O	1:A:131:GLU:HB2	2.16	0.45
1:A:151:LEU:CD2	1:A:156:LYS:HD3	2.46	0.45
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.45
1:A:40:ASN:HD21	1:A:119:LEU:HD21	1.82	0.45
1:A:193:TYR:CE2	1:A:297:ARG:HG3	2.52	0.45
1:A:392:ILE:O	1:A:396:VAL:HG23	2.17	0.44
1:A:74:LEU:HB2	1:A:77:GLU:HB2	1.99	0.44
1:A:3:GLU:CG	1:A:4:VAL:N	2.80	0.44
1:A:122:ASN:CG	1:A:123:GLU:H	2.20	0.44
2:A:601:HEM:CMA	8:A:620:CYS:HA	2.48	0.44
1:A:83:VAL:O	1:A:83:VAL:HG12	2.17	0.43
1:A:10:VAL:C	1:A:12:LEU:N	2.72	0.43
1:A:323:LYS:HB2	1:A:323:LYS:HE3	1.54	0.43
1:A:1:SER:O	1:A:2:TRP:C	2.56	0.43
2:A:601:HEM:HMA1	8:A:620:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:O	1:A:118:GLU:HB2	2.19	0.42
1:A:135:GLN:HB2	1:A:141:PRO:HD2	2.01	0.42
1:A:368:TRP:HZ3	1:A:389:ASP:OD1	2.03	0.42
1:A:17:GLU:CB	1:A:31:ARG:HE	2.32	0.42
1:A:255:ARG:HG2	8:A:620:CYS:CB	2.46	0.41
1:A:421:LEU:HB3	1:A:431:PHE:HB2	2.03	0.41
1:A:544:LEU:O	1:A:547:VAL:HG22	2.20	0.41
1:A:424:PRO:C	1:A:425:THR:HG23	2.40	0.41
1:A:8:ALA:CB	1:A:9:PRO:CD	2.96	0.41
1:A:122:ASN:CG	1:A:123:GLU:N	2.74	0.41
1:A:354:VAL:HG12	1:A:376:LEU:HD22	2.02	0.41
1:A:13:VAL:HG13	1:A:15:CYS:SG	2.61	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.95	0.41
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.21	0.41
1:A:371:GLU:CD	1:A:385:ARG:HH12	2.24	0.41
1:A:348:ARG:HD3	1:A:437:ASN:ND2	2.36	0.40
1:A:82:ILE:CD1	1:A:480:LEU:CD2	2.99	0.40
1:A:151:LEU:HD21	1:A:156:LYS:HD3	2.04	0.40
1:A:347:PHE:HB3	2:A:601:HEM:HMD3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/595 (100%)	558 (94%)	28 (5%)	6 (1%)	18 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLY
1	A	168	PRO

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Mol	Chain	Res	Type
1	A	171	PRO
1	A	123	GLU
1	A	170	PRO
1	A	427	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	498 (96%)	19 (4%)	39 33

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	12	LEU
1	A	32	ARG
1	A	52	GLU
1	A	63	GLN
1	A	64	ARG
1	A	71	ARG
1	A	124	HIS
1	A	125	SER
1	A	127	THR
1	A	141	PRO
1	A	172	TYR
1	A	220	TRP
1	A	270	LEU
1	A	282	LYS
1	A	334	SER
1	A	347	PHE
1	A	424	PRO
1	A	441	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	40	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	568	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	A	198	1	9,9,10	2.39	2 (22%)	9,12,14	3.46	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-N	-2.55	1.39	1.47
1	A	198	SEP	CA-C	5.97	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	-5.29	91.63	106.47
1	A	198	SEP	O2P-P-O1P	-2.31	101.46	110.50
1	A	198	SEP	O3P-P-OG	4.63	119.05	106.73
1	A	198	SEP	O2P-P-OG	6.63	124.39	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	614	1,5	14,14,15	1.01	0	15,19,21	1.66	7 (46%)
5	NAG	A	615	5	14,14,15	0.55	0	15,19,21	2.58	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	614	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	615	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	614	NAG	O4-C4-C3	-2.49	104.93	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	614	NAG	O7-C7-C8	-2.29	117.88	122.06
5	A	615	NAG	C6-C5-C4	-2.21	107.82	113.00
5	A	614	NAG	C1-C2-N2	2.03	113.95	110.49
5	A	614	NAG	O7-C7-N2	2.16	126.07	121.92
5	A	614	NAG	C2-N2-C7	2.29	126.29	122.94
5	A	615	NAG	C4-C3-C2	2.41	114.55	111.02
5	A	614	NAG	C1-O5-C5	2.44	115.53	112.17
5	A	614	NAG	C3-C4-C5	2.60	114.80	110.22
5	A	615	NAG	C3-C4-C5	3.03	115.56	110.22
5	A	615	NAG	C2-N2-C7	3.11	127.48	122.94
5	A	615	NAG	C1-O5-C5	7.68	122.75	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	601	9,1	28,50,50	2.33	10 (35%)	17,82,82	2.07	4 (23%)
6	NAG	A	616	1	14,14,15	0.54	0	15,19,21	0.98	1 (6%)
6	NAG	A	617	1	14,14,15	0.63	0	15,19,21	1.43	2 (13%)
6	NAG	A	618	1	14,14,15	0.62	0	15,19,21	1.31	0
7	SCN	A	619	-	1,2,2	0.84	0	0,1,1	0.00	-
8	CYS	A	620	-	2,6,6	4.34	2 (100%)	1,7,7	0.39	0
7	SCN	A	621	-	1,2,2	1.67	0	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	9,1	-	0/6/54/54	0/0/8/8
6	NAG	A	616	1	-	0/6/23/26	0/1/1/1
6	NAG	A	617	1	-	0/6/23/26	0/1/1/1
6	NAG	A	618	1	-	0/6/23/26	0/1/1/1
7	SCN	A	619	-	-	0/0/0/0	0/0/0/0
8	CYS	A	620	-	-	0/2/6/6	0/0/0/0
7	SCN	A	621	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-C2C	-6.76	1.31	1.40
8	A	620	CYS	CB-SG	-5.47	1.69	1.81
2	A	601	HEM	C4D-ND	-4.22	1.31	1.36
8	A	620	CYS	CB-CA	-2.78	1.49	1.53
2	A	601	HEM	CMD-C2D	2.02	1.55	1.51
2	A	601	HEM	CMA-C3A	2.43	1.56	1.51
2	A	601	HEM	CAA-C2A	2.46	1.56	1.52
2	A	601	HEM	CAD-C3D	2.59	1.57	1.52
2	A	601	HEM	CMC-C2C	2.71	1.57	1.51
2	A	601	HEM	C3D-C2D	2.73	1.45	1.37
2	A	601	HEM	C3C-CAC	3.71	1.55	1.47
2	A	601	HEM	C3B-CAB	4.04	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CAD-CBD-CGD	-5.14	103.87	112.66
2	A	601	HEM	CBD-CAD-C3D	-3.92	104.99	112.47
6	A	617	NAG	C1-C2-N2	-3.57	104.39	110.49
2	A	601	HEM	C1D-C2D-C3D	-2.84	105.02	107.00
6	A	616	NAG	C3-C4-C5	-2.70	105.46	110.22
6	A	617	NAG	O5-C1-C2	-2.46	108.05	111.47
2	A	601	HEM	CAA-C2A-C3A	-2.11	122.99	129.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	4	0
8	A	620	CYS	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	594/595 (99%)	1.04	61 (10%) 7 9	20, 37, 79, 109	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	15.9
1	A	121	SER	13.1
1	A	124	HIS	12.2
1	A	10	VAL	11.5
1	A	594	GLU	10.5
1	A	593	ARG	10.1
1	A	119	LEU	9.8
1	A	7	GLY	9.2
1	A	122	ASN	8.7
1	A	595	ASN	8.5
1	A	8	ALA	7.9
1	A	4	VAL	7.8
1	A	123	GLU	7.5
1	A	167	CYS	7.2
1	A	172	TYR	7.2
1	A	5	GLY	6.3
1	A	120	GLY	5.9
1	A	13	VAL	5.8
1	A	592	SER	5.8
1	A	9	PRO	5.4
1	A	14	LYS	4.7
1	A	171	PRO	4.6
1	A	11	PRO	4.5
1	A	16	ASP	3.7
1	A	173	GLN	3.6
1	A	582	VAL	3.4
1	A	220	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	209	PRO	3.3
1	A	231	ASN	3.2
1	A	1	SER	3.2
1	A	170	PRO	3.0
1	A	12	LEU	3.0
1	A	132	TYR	2.9
1	A	126	LYS	2.9
1	A	169	THR	2.8
1	A	3	GLU	2.8
1	A	175	LEU	2.8
1	A	18	ASN	2.7
1	A	131	GLU	2.7
1	A	223	GLY	2.6
1	A	441	CYS	2.6
1	A	168	PRO	2.5
1	A	174	SER	2.5
1	A	208	SER	2.5
1	A	161	PHE	2.5
1	A	17	GLU	2.4
1	A	117	THR	2.4
1	A	125	SER	2.4
1	A	64	ARG	2.3
1	A	127	THR	2.3
1	A	6	CYS	2.3
1	A	130	GLU	2.2
1	A	425	THR	2.2
1	A	559	ILE	2.2
1	A	544	LEU	2.2
1	A	242	THR	2.1
1	A	269	LEU	2.1
1	A	591	ALA	2.1
1	A	210	LEU	2.1
1	A	587	LEU	2.1
1	A	277	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy

less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	A	198	10/11	0.94	0.18	-	27,41,44,48	0

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	614	14/15	0.88	0.16	0.42	24,29,38,38	0
5	NAG	A	615	14/15	0.75	0.26	-	51,59,62,63	0

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CYS	A	620	7/7	0.89	0.28	12.19	22,36,38,40	0
6	NAG	A	618	14/15	0.85	0.28	2.20	40,45,54,55	0
7	SCN	A	621	3/3	0.94	0.21	1.79	48,48,49,49	0
4	IOD	A	606	1/1	1.00	0.15	-0.11	19,19,19,19	0
6	NAG	A	616	14/15	0.90	0.15	-0.65	22,30,36,39	0
7	SCN	A	619	3/3	0.94	0.14	-0.75	9,9,12,14	0
2	HEM	A	601	43/43	0.96	0.12	-1.54	10,15,22,24	0
4	IOD	A	608	1/1	0.96	0.09	-1.85	37,37,37,37	0
3	CA	A	602	1/1	0.99	0.08	-3.14	17,17,17,17	0
4	IOD	A	604	1/1	0.98	0.03	-3.91	42,42,42,42	0
4	IOD	A	603	1/1	0.99	0.04	-4.62	34,34,34,34	0
4	IOD	A	605	1/1	0.98	0.04	-5.05	31,31,31,31	0
4	IOD	A	607	1/1	0.98	0.06	-5.83	27,27,27,27	0
4	IOD	A	610	1/1	0.94	0.07	-	70,70,70,70	0
4	IOD	A	609	1/1	0.94	0.04	-	47,47,47,47	0
6	NAG	A	617	14/15	0.80	0.22	-	39,44,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IOD	A	612	1/1	0.89	0.14	-	62,62,62,62	0
4	IOD	A	611	1/1	0.97	0.12	-	45,45,45,45	0
4	IOD	A	613	1/1	0.96	0.09	-	68,68,68,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.